Estimating Derivatives and Richardson Extrapolation

Suppose we want to approximate \( f'(x) \) using values of \( f \) only. The natural approach would be to compute

\[
    f'(x) \approx \frac{f(x+h) - f(x)}{h}
\]

for some small \( h \).

We can find the error in this approximation using Taylor's theorem:

\[
f(x+h) = f(x) + f'(x)h + \frac{1}{2}h^2 f''(\xi)
\]

or

\[
f(x+h) - f(x) - \frac{1}{2}h^2 f''(\xi) = f'(x)h
\]

or

\[
f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2}h f''(\xi).
\]

This implies that the error is \( O(h) \).
Can we improve on this situation? Consider the Taylor series
\[ f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \ldots \]
\[ f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \ldots \]
If we subtract, we get
\[ f(x+h) - f(x-h) = 2hf'(x) + \frac{1}{3}h^3f'''(x) + \ldots \]
so
\[ f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}h^2f'''(x) + \ldots \]
This is clearly better, since the error is \( O(h^2) \) rather than \( O(h) \).
We can actually rewrite the error term as \(-\frac{1}{6}h^2 f'''(\xi)\) for some \(\xi\) in the interval \([x-h, x+h]\).

\(<\text{derivative}_{\text{-}}\text{and}\text{-}\text{difference}_{\text{-}}\text{-2}_{\text{.}}\text{nb}\)>

As we can see, this works considerably better! Now here is a very clever idea. Observe that our previous subtraction

\[
\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2 c}{2} + \frac{h^4 d}{24} + \ldots
\]

or

\[
f'(x) = \frac{f(x+h) - f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + \ldots
\]

since all of the odd power terms have cancelled each other out.
Now suppose we write

\[ \varphi(h) = \frac{f(x+h) - f(x-h)}{2h} \]

\[ = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots \]

It is clear that as \( h \to 0, \varphi(h) \to f'(x) \).

But consider the relationship between \( \varphi(h) \) and \( \varphi(h/2) \).

\[ \varphi(h) = f'(x) - a_2 \frac{h^2}{4} - a_4 \frac{h^4}{16} - a_6 \frac{h^6}{64} - \ldots \]

\[ \varphi(h/2) = f'(x) - a_2 \frac{h^2}{4} - a_4 \frac{h^4}{16} - a_6 \frac{h^6}{64} - \ldots \]

This means that

\[ \varphi(h) - 4 \varphi(h/2) = -3f'(x) - \frac{3}{4} a_4 h^4 - \frac{15}{16} a_6 h^6 - \ldots \]

and so forth. Now we can get

\[ -\frac{1}{3} \varphi(h) + \frac{4}{3} \varphi(h/2) = f'(x) + \frac{31}{4} a_4 h^4 + \frac{35}{16} a_6 h^6 + \ldots \]

\[ \varphi(h/2) + \frac{1}{3} [\varphi(h) - \varphi(h)] = \]
We have now improved our error bound to $O(h^4)$ just by adding a correction term of $\frac{1}{3} [\Phi(h) - \Phi(h)]$ to $\Phi(h)$. This is shocking!

And we can play this game again. Let

$$\Phi(h) = \frac{1}{3} \Phi(h) - \frac{1}{3} \Phi(h).$$

Then for some coefficients $b_i$,

$$\Phi(h) = f'(x) + b_4 h^4 + b_6 h^6 + \ldots,$$

$$\Phi(h) = f'(x) + b_4 \frac{h^4}{16} + b_6 \frac{h^6}{64} + \ldots,$$

so

$$\Phi(h) - 16 \Phi(h) = -15 f'(x) + \frac{3}{4} b_6 h^6 + \ldots$$

or

$$\Phi(h) + \frac{1}{15} [\Phi(h) - \Phi(h)] = f'(x) - \frac{1}{20} b_6 h^6 + \ldots$$
This procedure is called Richardson extrapolation.

We can formalize the procedure inductively as follows. Suppose

\[ \Phi(h) = L - \sum_{k=1}^{\infty} a_{2^k} h^{2^k} \]

and we want to compute \( L \) by computing \( \Phi(h) \) at various \( h \) values.

For some given \( h \), compute

\[ D(n,0) = \Phi\left(\frac{h}{2^n}\right), \quad n \geq 0 \]

We know

\[ D(n,0) = L + \sum_{k=1}^{\infty} A(k,0) \left(\frac{h}{2^n}\right)^{2^k} \]

where the \( A(i,j) \) are unknown coefficients.
We define
\[ D(n, m) = \frac{4^m}{4^{m-1}} D(n, m - 1) - \frac{1}{4^{m-1}} D(n-1, m-1). \]

Claim.
\[ D(n, m) = L + \sum_{k=m+1}^{8} A(k, m) \left( \frac{h}{2^n} \right)^{2k} \]

We will now prove this by induction on \( m \).
For \( m = 0 \), there's nothing to check, so assume this holds for \( m - 1 \). Then
\[ D(n, m) = \frac{4^m}{4^{m-1}} \left[ L + \sum_{k=m}^{8} A(k, m - 1) \left( \frac{h}{2^n} \right)^{2k} \right] \]
\[ - \frac{1}{4^{m-1}} \left[ L + \sum_{k=m}^{8} A(k, m - 1) \left( \frac{h}{2^{n-1}} \right)^{2k} \right]. \]
\[
= L + \sum_{k=m}^{\infty} A(k, m-1) \frac{y^m - 2^k}{y^m - 1} \left( \frac{h}{2^n} \right)^{2k}
\]

So we can define

\[
A(k, m) = A(k, m-1) \left( \frac{y^m - 2^k}{y^m - 1} \right) \quad \text{this is } < 1.
\]

Since

\[
A(m, m) = 0,
\]

we can write

\[
D(n, m) = L + \sum_{k=m+1}^{\infty} A(k, m) \left( \frac{h}{2^n} \right)^{2k}, \quad \Box
\]

We then compute

\[
\begin{align*}
D(0, 0) & \leftarrow \\
D(1, 0) & \leftarrow D(1, 1) \\
D(2, 0) & \leftarrow D(2, 1) \leftarrow D(2, 2)
\end{align*}
\]
To see what this looks like in practise we turn to

<richardson-extrapolation.nb>

The next general plan for computing derivatives is to fit a polynomial through some points near \( x \) and differentiate the polynomial instead.

Our previous pictures should convince you that this is dangerous!